

# Canted spiral magnetic order in layered systems

TIMIRGAZIN Marat <sup>a</sup>, GILMUTDINOV Vitaly <sup>b</sup>, and ARZHNIKOV Anatoly <sup>c</sup>

Physical-Technical Institute, Ural Branch of Russian Academy of Sciences, Kirova str. 132, Izhevsk  
426000, Russia

<sup>a</sup>timirgazin@gmail.com, <sup>b</sup>vitaliodestroyer@gmail.com, <sup>c</sup>arzhnikof@bk.ru

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**Abstract.** Formation of a canted spiral magnetic order is studied in the framework of a mean-field approximation of the Hubbard model. It is revealed that this magnetic state can be stabilized under certain conditions in layered systems with a relatively small interplane electron hopping. Example of an experimentally observed magnetic structure of  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  is considered. It is shown that the canting magnetic order can be described in terms of a simple non-relativistic band magnetism.

## Introduction

It is generally accepted that interplay between charge carriers and magnetic correlations is responsible for high-temperature superconductivity in cuprates. Magnetic structure forms an environment for hole motion, and determination of its characteristics and of its evolution with doping is therefore very important problem in clarifying the mechanism of superconductivity.

Parent  $\text{CuO}_2$ -based compounds, e.g.  $\text{La}_2\text{CuO}_4$ , are quasi-two-dimensional Heisenberg antiferromagnets. With doping of Sr atoms, the magnetic structure of  $\text{La}_2\text{CuO}_4$  significantly changes. Presence of additional holes favors incommensurate spin density waves formation. Neutron scattering in  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  reveals coexistence of both commensurate and incommensurate magnetic structures in the vicinity of half-filling (hole doping  $x < 0.02$ ) [1]. At  $x \sim 0.02$  the system goes to the incommensurate (spin glass) state with the magnetic structure wave vector  $\mathbf{Q} = (Q, Q)$ . For  $x > 0.06$  a magnetic structure with the wave vector  $\mathbf{Q} = (Q, \pi)$  is stabilized [2].

Theoretical calculations based on Hartree-Fock and slave-boson approaches in the Hubbard model confirm the formation of incommensurate (spiral) magnetic structures with the hole doping [3, 4, 5, 6]. Phase diagrams of the 2D Hubbard model for the relation of next-nearest neighbor hopping to nearest neighbor hopping  $t'/t = 0.2$ , which approximately corresponds to  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  [7], qualitatively fully reproduce the magnetic phase transitions observed in experiment with doping [5, 6].

The in-plane antiferromagnetic exchange interaction between Cu atoms is typically  $J_{\parallel} \sim 0.1\text{eV}$ , as was determined by inelastic neutron scattering [8] and by Raman scattering. Weak interaction between the  $\text{CuO}_2$  layers (interplane exchange interaction is estimated to be  $J_{\perp} \sim 10^{-5}J_{\parallel}$  [9]) gives rise to the three-dimensional long-range Néel order ( $T_N \approx 325\text{K}$ ) [10, 11]. Additionally, each CuO plane has a weak perpendicular magnetic moment, and the interplane exchange orients these moments antiferromagnetically as shown in Fig. 1a. The spins, hence, are canted  $0.17^\circ$  away from  $xy$ -plane [12]. The canting is shown to persist with a light doping of Sr ( $x = 0 - 0.03$ ) [13]. The authors of [13] note an unusual susceptibility anisotropy observed in doped region, which can be explained by a spin-density wave magnetic structure. The resulting

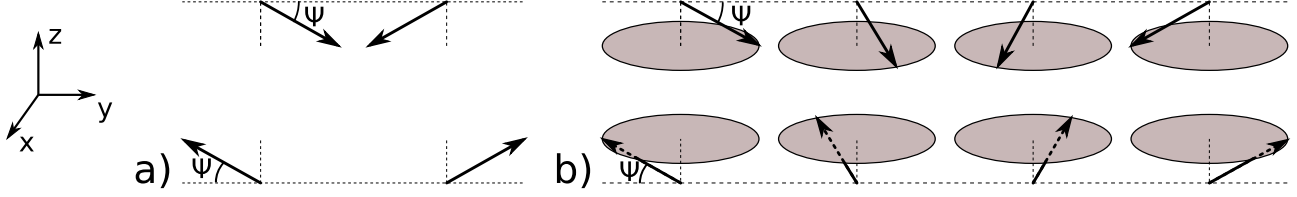


Fig. 1: Sketch of a 3D canted spin order: a) antiferromagnetic in  $\text{La}_2\text{CuO}_4$  b) spiral in  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ . The canting angle  $\psi$  from the  $xy$  CuO planes is exaggerated.

supposed magnetic structure of  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  can then be presented as a combination of the spiral type of spin-density wave with a canting (Fig. 1b.).

The canting is traditionally associated with a Dzyaloshinskii-Moriya interaction which is appeared due to orthorhombic structure in  $\text{La}_2\text{CuO}_4$ . In the current work we study another scenario of such magnetic structure formation, which is based only on simple Hubbard model assumptions and does not require spin-orbit coupling. For this we use the 3D Hubbard model taking into account spiral magnetic states, with the interplane electron hopping much smaller than the in-plane hopping.

## Formalism

The Hubbard Hamiltonian of the considered layered system is divided into the kinetic energy of electrons hopping between sites  $K$ , and the repulsive Coulomb on-site interaction  $V$ :

$$\mathcal{H} = K + V = \sum_{\langle\alpha,\beta\rangle,\langle i,j\rangle,\sigma} t_{\alpha,\beta,i,j} c_{\alpha,i,\sigma}^\dagger c_{\beta,j,\sigma} + U \sum_{\alpha,j} n_{\alpha,j,\uparrow} n_{\alpha,j,\downarrow}, \quad (1)$$

where  $\langle\alpha,\beta\rangle = 1, 2$  are numbers of planes,  $\langle i,j\rangle$  are in-plane site numbers,  $\sigma$  is spin number.

We suppose the interplane transfer integral  $t_z$  to be much smaller than the in-plane transfer integral  $t_{xy}$ . After Fourier transformations  $K$  takes the form:

$$K = \sum_{\alpha,\mathbf{k},\sigma} \varepsilon_{\mathbf{k}}^{xy} c_{\alpha,\mathbf{k},\sigma}^\dagger c_{\alpha,\mathbf{k},\sigma} + \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}}^z (c_{1,\mathbf{k},\sigma}^\dagger c_{2,\mathbf{k},\sigma} + c_{2,\mathbf{k},\sigma}^\dagger c_{1,\mathbf{k},\sigma}), \quad (2)$$

where  $\varepsilon_{\mathbf{k}}^{xy} = -2t_{xy}(\cos k_x + \cos k_y) + 4t'_{xy} \cos k_x \cos k_y$  and  $\varepsilon_{\mathbf{k}}^z = -2t_z \cos k_z$  are the in-plane and interplane dispersion laws. Nearest and next-nearest neighbors electron hopping is taken into account in plane.

Interaction term  $V$  can be written in terms of electron and spin densities using  $n_\uparrow n_\downarrow = n^2/4 - \mathbf{S}^2$ . Then in the mean-field (Hartree-Fock) approximation:

$$V = UN \left( M^2 - \frac{n^2}{4} \right) + 2U \sum_{\alpha,j} \left( \frac{n}{4} n_{\alpha,j} - \mathbf{M}_{\alpha,j} \mathbf{S}_{\alpha,j} \right), \quad (3)$$

where  $n = \langle n_{\alpha,i} \rangle$  is a uniform average electron concentration,  $\mathbf{M}_{\alpha,j} = \langle \mathbf{S}_{\alpha,j} \rangle$  is average magnetization,  $M$  is its amplitude,  $N$  is full number of sites in the system.

The magnetic structure depicted on Fig.1b is described by following vector:

$$\mathbf{M}_{\alpha,j} = (M \cos \mathbf{QR}_j \cos \psi, M \sin \mathbf{QR}_j \cos \psi, M(-1)^{\alpha+1} \sin \psi), \quad (4)$$

with  $\mathbf{Q}$  being the in-plane wave vector. Taking this into account, we obtain:

$$V = UN \left( M^2 - \frac{n^2}{4} \right) + \frac{Un}{2} \sum_{\alpha,j} n_{\alpha,j} - UM \sum_{\alpha,j} (S_{\alpha,j}^+ e^{-i\mathbf{Q}\mathbf{R}_j} \cos \psi + S_{\alpha,j}^- e^{i\mathbf{Q}\mathbf{R}_j} \cos \psi + 2S_{\alpha,j}^z (-1)^{\alpha+1} \sin \psi) \quad (5)$$

In  $k$ -space, we have:

$$V = UN \left( M^2 - \frac{n^2}{4} \right) + \frac{Un}{2} \sum_{\alpha,\mathbf{k},\sigma} c_{\alpha,\mathbf{k},\sigma}^\dagger c_{\alpha,\mathbf{k},\sigma} - UM \sum_{\alpha,\mathbf{k}} (c_{\alpha,\mathbf{k},\uparrow}^\dagger c_{\alpha,\mathbf{k}+\mathbf{Q},\downarrow} \cos \psi + c_{\alpha,\mathbf{k}+\mathbf{Q},\downarrow}^\dagger c_{\alpha,\mathbf{k},\uparrow} \cos \psi + (c_{\alpha,\mathbf{k},\uparrow}^\dagger c_{\alpha,\mathbf{k},\uparrow} - c_{\alpha,\mathbf{k}+\mathbf{Q},\downarrow}^\dagger c_{\alpha,\mathbf{k}+\mathbf{Q},\downarrow}) (-1)^{\alpha+1} \sin \psi). \quad (6)$$

Full Hamiltonian (1) represents a quadratic form of creation and annihilation operators  $c_{1,\mathbf{k},\uparrow}$ ,  $c_{1,\mathbf{k}+\mathbf{Q},\downarrow}$ ,  $c_{2,\mathbf{k},\uparrow}$ ,  $c_{2,\mathbf{k}+\mathbf{Q},\downarrow}$ . To diagonalize the Hamiltonian, one must solve a polynomial equation of 4-th degree. We have used the Ferrari's method for this and have found eigenvalues  $\varepsilon_{\mathbf{k},l}$  and eigenvectors  $T_{\mathbf{k},lm}$  in each  $k$ -point. The electron concentration  $n$ , magnetic moment  $M$  and total energy  $E$  can be expressed as:

$$n = \frac{1}{N} \sum_{\mathbf{k},l} f(\varepsilon_{\mathbf{k},l}), \quad (7)$$

$$M = \frac{1}{N \cos \psi} \sum_{\mathbf{k},l} (T_{\mathbf{k},1l}^* T_{\mathbf{k},2l} + T_{\mathbf{k},3l}^* T_{\mathbf{k},4l}) f(\varepsilon_{\mathbf{k},l}), \quad (8)$$

$$E = UN \left( M^2 - \frac{n^2}{4} \right) + \sum_{\mathbf{k},l} \varepsilon_{\mathbf{k},l} f(\varepsilon_{\mathbf{k},l}), \quad (9)$$

where  $f(\varepsilon_{\mathbf{k}l})$  is the Fermi function.

In order to obtain the ground state of the system for given parameters  $n, U, t_{xy}, t'_{xy}, t_z$  the total energy should be minimized with respect to all  $\mathbf{Q}$  and  $\psi$ .

## Results

The magnetic phase diagram of the ground state of the 2D Hubbard model in Hartree-Fock approximation for  $t' = 0.2$ , which approximately corresponds to real  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  value, was calculated in [5] (Fig. 3a in reference). Our investigation is focused on hole-doped side of this diagram which contains  $(Q, Q)$  and  $(Q, \pi)$  spiral magnetic, ferromagnetic, and antiferromagnetic phases. The values of  $U/t$  studied, approximately correspond to realistic values of  $U/t$  for cuprates which lie in the range  $8 - 20$  according to the ab initio calculations [14]. The value of  $t_z$  is taken to be  $0.1t_{xy}$ .

We considered both  $(Q, Q)$  and  $(Q, \pi)$  spiral states to determine if the addition of the weak interplane electron hopping can stabilize the canted spiral magnetic order. Technically, this is reduced to finding (for some parameters  $U/t, n$ ) a  $Q$  value that minimizes the energy (9) with  $\psi = 0$  for each direction of  $\mathbf{Q}$  vector, and next to finding a  $\psi$  angle that minimizes the energy (9) for this  $Q$ .

Our investigation shows that the canting is not energetically favorable for the  $(Q, Q)$  state for all the parameters studied. But for the  $(Q, \pi)$  phase this is not the case. In Fig. 2 the dependence

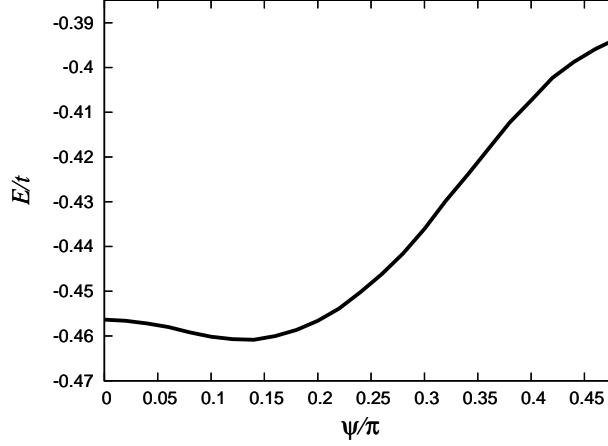


Fig. 2: Dependence of the total energy  $E$  upon the canting angle  $\psi$  for  $U/t_{xy} = 10, n = 0.9, t'_{xy} = 0.2, t_z = 0.1, \mathbf{Q} = (0.65\pi, \pi)$ .

of the total energy  $E$  upon the canting angle  $\psi$  for  $U/t_{xy} = 10, n = 0.9, \mathbf{Q} = (0.65\pi, \pi)$  is presented. The minimum of energy corresponds to  $\psi = 0.14\pi$ , which means that the canted spiral state is the most energetically favorable among the  $(Q, \pi)$  states at these parameters. It should be noted that this is not the ground state because the phase separation between  $AF$  and  $FM$  phases is still more favorable, as in the 2D system [5].

Our result can be qualitatively associated with the results of paper [15], where stability of  $(Q, Q)$  and  $(Q, \pi)$  phases in respect to transverse spin fluctuations was studied for small  $t'/t$  and hole doping. It was found that from these two states only  $(Q, \pi)$  is unstable and tends to form a non-coplanar spin configuration.

The results obtained show a possibility of stabilization of the canted spiral magnetic state in the systems with weakly coupled layers in the simple Hubbard model without account of spin-orbit interaction. So, we have demonstrated an alternative non-relativistic scenario of formation of the canted magnetic structure which is not based on the Dzyaloshinskii-Moriya interaction.

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## References

- [1] M. Matsuda, M. Fujita, K. Yamada, R. J. Birgeneau, Y. Endoh, and G. Shirane: Phys. Rev. B Vol. 65 (2002), p. 134515
- [2] M. Fujita, K. Yamada, H. Hiraka, P. M. Gehring, S. H. Lee, S. Wakimoto, and G. Shirane: Phys. Rev. B Vol. 65 (2002), p. 064505
- [3] S. Sarker, C. Jayaprakash, H.R. Krishnamurthy and W. Wenzel: Phys. Rev B Vol. 43 (1991), p. 8775
- [4] R. Fresard and P. Wölfle, J. Phys.: Cond. Matt. Vol. 4 (1992), p. 3625

- [5] P. A. Igoshev, M. A. Timirgazin, A. A. Katanin, A. K. Arzhnikov and V. Yu. Irkhin: Phys. Rev. B Vol. 81 (2010), p. 094407
- [6] P.A. Igoshev, M.A. Timirgazin, A.K. Arzhnikov and V.Yu. Irkhin: JETP Letters Vol. 98 (2013), p. 150
- [7] M.S. Hybertsen, E.B. Stechel, W.M.C. Foulkes and M. Schlter: Phys. Rev. B Vol. 45 (1992), p. 10032
- [8] R.J. Birgeneau, Y. Endoh, K. Kakurai, Y. Hidaka, T. Murakami, M.A. Kastner, T.R. Thurston, G. Shirane and K. Yamada: Phys. Rev. B Vol. 39 (1989), p. 2868
- [9] S-W. Cheong, Z. Fisk, J.O. Willis, S.E. Brown, J.D. Thompson, J.P. Remeik, A.S. Cooper, R.M. Aikin, D. Schiferl, G. Gruner: Solid State Comm. Vol. 65 (1988), p. 111
- [10] B. Keimer, N. Belk, R.J. Birgeneau, A. Cassanho, C.Y. Chen, M. Greven, M.A. Kastner, A. Aharony, Y. Endoh, R.W. Erwin, and G. Shirane: Phys. Rev. B Vol. 46 (1992), p. 14034
- [11] M.A. Kastner, R.J. Birgeneau, G. Shirane and Y. Endoh: Rev. Mod. Phys. Vol. 70 (1998), p. 897
- [12] T. Thio, T.R. Thurston, N.W. Preyer, P.J. Picone, M.A. Kastner, H.P. Jenssen, D.R. Gabbe, C.Y. Chen, R.J. Birgeneau and A. Aharony: Phys. Rev. B Vol. 38 (1988), p. 905
- [13] A.N. Lavrov, Y. Ando, S. Komiya and I. Tsukada: Phys. Rev. Lett. Vol. 87 (2001), p. 017007
- [14] S. Hybertsen, E.B. Stechel, M. Schluter, and D.R. Jennison: Phys. Rev. B Vol. 41 (1990), p. 11068
- [15] A.V. Chubukov and K.A. Musaelian: Phys. Rev. B Vol. 51 (1995), p. 12605